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Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding

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ABSTRACT

We studied the use of online molecular dynamics simulations (MD) to enhance student abilities to understand the atomic processes governing plastic deformation in materials. The target population included a second-year undergraduate engineering course in the School of Materials Engineering at Purdue University. The objectives of the study were to help students (i) understand the atomic-level processes that govern plastic deformation in metals, and (ii) develop a more intuitive understanding of how materials look and behave in atomic scales. The treatment consisted of traditional lectures followed by inquiry-based simulation lab activities powered by research-grade computational tools. Two lectures by the instructor reviewed the topic of plastic deformation and presented the basic physics of modeling MD to provide a description of materials with atomic resolution of the forces. Next, the students used a simulated laboratory experience to conduct several inquiry activities using fully interactive online MD simulations. Students needed to use the visualizations provided by the simulation to evaluate the atomic processes responsible for plastic deformation of materials and they computed values of various materials properties. Our first analysis compared differences between students who attended one or two lectures and those who attended no lectures. The results showed that participation in the background and/or pre-laboratory lectures supported student abilities to recall specific facts and behavior of materials explicitly taught during instruction. The lectures did not prepare most students for transferring what they had learned in the lecture or prelab lectures to problems they had not previously encountered, but were first presented in the laboratory activities. However, most students who participated in the laboratory experience demonstrated the ability to transfer what they had learned to predict how an unfamiliar material would behave at the molecular level. This instructional approach can be generalized to other learning experiences designed to help students apply abstract fundamental engineering principles to evaluate a larger context of unfamiliar situations.

Keywords: simulations, molecular dynamics, materials

INTRODUCTION

Modeling and simulation are fundamental tools used in engineering to comprehend the behavior of complex concepts and to predict the behavior of new designs. Computational simulation tools can output a wide range of representations of information. This information combined with the learner's goals to answer questions can lead to a learner's construction of knowledge they can transfer to new situations. For example, data can be visualized with graphs illustrating relationships between two variables that influence the behavior of a system. These graphs can describe and predict how a system will change as one of these factors changes. Or pictures and animations can illustrate the spatial configuration of a system (such as a device or material). Simulation tools can dynamically generate data and represent it with graphs and/or a collection of images. Researchers use simulation tools to help make sense of complex ideas when they design devices and build theories to improve the descriptive models defining the behavior of these simulations.

We hypothesized that undergraduate engineering students can use these tools to develop their conceptual understanding of how a system works and the multitude of factors that govern how it behaves. This knowledge provides them with an important mental representation they can use to predict the performance of a system under conditions that they did not experience firsthand. In this study we provide a description of an instructional initiative that uses online molecular dynamics (MD) simulation to develop students' conceptual understanding of how materials behave at the atomic level. The simulation provides a graph of stress versus strain and a visualization of interactive atomic snapshots of the state of the system at various stages of deformation. Incorporating advanced simulations in undergraduate education requires no expertise in scientific computing or specialized equipment; nanoHUB.org (a web portal developed by the Network for Computational Nanotechnology with support from the U.S. National Science Foundation) enables users worldwide to perform online simulations, free of charge, by simply using a web browser (Strachan, Klimeck, and Lundstrom 2010) to facilitate the incorporation of online atomistic simulations in materials education, We designed and deployed a learning module consisting of audiovisual lectures, including a tutorial on online MD simulations and hands-on activities; this module is available at https://nanohub.org/topics/LearningModulePlasticityMD. The nanoHUB also provides a search capability to find this module on molecular dynamics and many related resources the reader will find useful.

We begin this paper with a description of the need for computational programs in engineering and how simulation was used in a second-year undergraduate materials engineering course. Next we briefly describe the underlying theory of how students reason with these tools in a way that develops their abilities to predict how a material will behave in a context that was not explicitly taught during either a background lecture or prelab lecture, or both. We conclude with a description of the methods and results detailing what students learned through their interaction with the simulation learning experience.

Molecular Dynamic Simulations of Material Structures

Modeling and simulation of materials are important skills for both undergraduate and graduate students in materials science engineering for the design and optimization of materials (Thornton and Asta 2005). This is critical whether they are trying to select a material for their design of a product or whether they are designing a new material. The Accreditation Board for Engineering and Technology (ABET 2009) define criteria for engineering programs, including studies of materials, materials processing, ceramics, glass, polymer, and metallurgy, plus the appropriate applications of experimental, statistical, and computational methods to solve materials selection and design problems. Furthermore, the National Research Council (2008) emphasized that an integrated computational materials engineering curriculum can accelerate materials development, transform the engineering design optimization process, and unify design and manufacturing. Based on these needs, the incorporation of computational methods has been an integral component of many materials science engineering programs, including our school of materials engineering at Purdue University. One of the most challenging topics undergraduate materials science engineering students face in their studies is the relationship between atomic structure and processes combined with the resulting macroscopic materials response (similar complex interactions in other domains described by Arcavi 2003; Edelson and Gordin 1998; Pea 1987). Also, Rudnyi and Korvink (2003) argued that engineers have little experience with molecule-oriented problems, and we believe the inquiry processes used to investigate this abstract domain with computational skills is important for all engineering disciplines. MD simulations provide detailed and accurate models for developing conceptual understanding of materials from the bottom up. As part of introductory material science engineering courses, for example, students learn about dislocations as the defects responsible for plastic deformation in many crystalline materials and their interaction with other lattice defects as strengthening mechanisms.

This bottom-up approach (atomic to macro scale) is important as nanoscience and nanotechnology drive the characteristic size of many materials and devices to the nanoscale level in search of improved material performance. Materials engineers and scientists have traditionally built upon an understanding of the atomic and molecular processes governing the performance of materials to design and optimize them for a range of conditions. This conceptual framework is how materials science and engineering is taught and learned; students are introduced to atomic processes and phenomena early on in their undergraduate studies.

Traditional instruction of material structures visualizes at the atomic level through the use of static two-dimensional (2-D) images depicting 3-D orientation of the structures. These static images and graphs, combined with narrative descriptions in textbooks and didactic lectures, describe how the structures change under various loading conditions (tension and compression). These descriptions are often coupled with laboratory demonstrations of a material undergoing tensile axial loading, if a university has the facilities to conduct such experiments. Figure 1 illustrates a common test configuration for loading a material in either tension or compression (many video examples of this kind of test can be found on YouTube.com). Figure 2 illustrates a common graphical representation used to illustrate the result of such experiments; it shows the relationship between stress and strain of a material in tensile loading. Empirical tests are performed on various materials to determine these unique relationships between stress and strain. Images like these can be very expressive and support students' understanding of the basic properties of materials and critical events when the materials properties are permanently changed. The loading conditions of a material prior to the yield stress

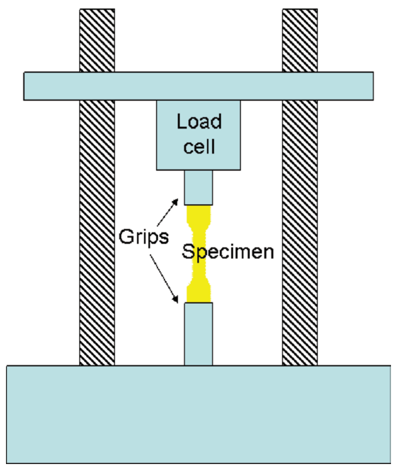

Figure 1. Specimen in tensile test

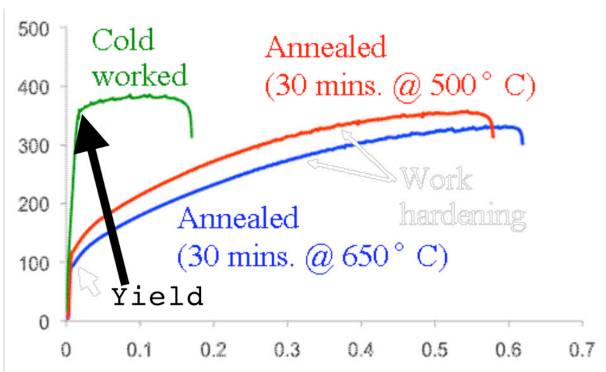

Figure 2. Stress v. Strain relationship

will lead to no permanent deformation of a material. Therefore the atomic structure of the material does not change. However, when the external load applied to the specimen exceeds the yield stress, irreversible atomic processes occur that lead to a permanent change in shape. Thus the yield stress is an extremely important property for materials engineers. For purposes of comparison, we consider this traditional demonstration as a macro-level physical experiment to illustrate the plastic deformation of a material under various loading conditions.

As part of a second-year undergraduate laboratory course in materials structure and properties, we have been exploring the potential of using MD simulations coupled with highly expressive scientific visualizations illustrating atomic structures to improve learners' conceptual understanding of materials and their behavior at the atomic scale. This initiative is designed to complement the experimental tests students carry out in the course and represents a computational experiment to illustrate the plastic deformation of a material.

MD simulations provide a very detailed description of material behavior by numerically solving the dynamics of every single atom in the specimen; i.e., the result of the simulation is the position and velocity of every atom as a function of time. Having second-year engineering students perform MD simulations without training in scientific computing is facilitated with a U.S. National Science Foundation web portal, nanoHUB.org, which enables users to run live online simulation tools using only a web browser. This portal was developed at Purdue University by the Network for Computational Nanotechnology and provides access to research grade simulations, with highly expressive visualizations, for the performance of computational experiments. Scientists and engineers use these tools to publicize their theories and engineering design decisions. Educators in engineering and science, however, have been using nanoHUB.org simulation tools for graduate and undergraduate education for a range of engineering and scientific investigations and learning goals (Magana 2009; Magana, Brophy, and Bodner, 2012, 2009, 2008). For example, some instructors of undergraduate students use simulations to demonstrate physical phenomena to learn governing principles associated with their area of science. In this context, the simulation represents natural phenomena that students can explore through scientific inquiry.

For the hands-on activities, we used the nanoMATERIALS Simulation Tool (Strachan et al. 2006), a general purpose MD code (computational model) available at nanoHUB.org. We believe that comparing the dynamic demonstrations at the atomic level with macro-level demonstrations provides a robust method for supporting learners' comprehension of material behavior. Further, student interactions with the model were designed to facilitate their noticing the structural changes governing plastic deformation in nanoscale specimens and their ability to use this knowledge to predict the behavior of other materials. This level of knowledge is more likely to transfer to subsequent situations involving new materials under loading conditions because students are engaged in providing

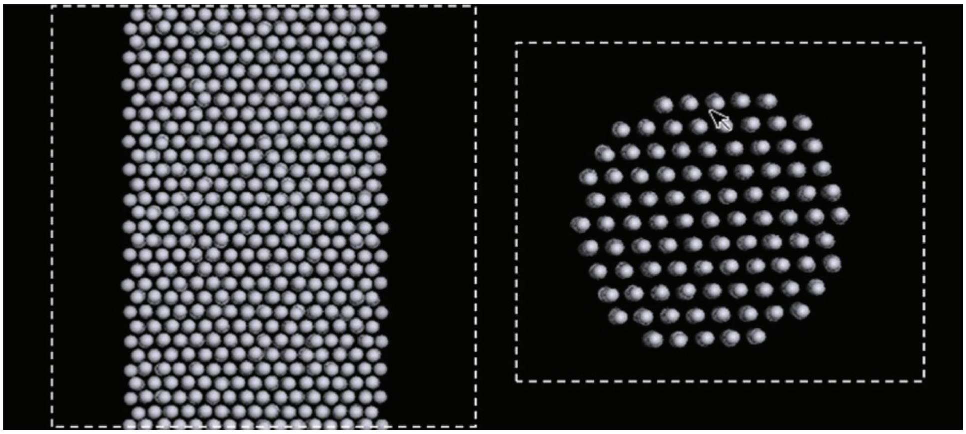

Figure 3. Side and cross-sectional view of the atomic structure of a nanowire

explanations of how materials behave as a goal of their inquiry with a virtual laboratory (analogous to other transfer conditions described by Bransford and Schwartz, 2000). For example, part of the computational model is the atomic structure of a material under investigation. Figure 3 illustrates two views of an image obtained from the MD computational simulation depicting the atomic structure of a nanowire. The second view in Figure 3 illustrates the image rotated to view the cross-sectional area of the structure.

Running the nanoMATERIALS simulation tool, produces 3-dimensional images that the students can inspect by rotating and zooming with simple mouse interface manipulations. These images are generated based on the initial conditions students specify. They can evaluate these images to see how the material changes its structure over time as an external force is applied similar to the macro-level experiment. As shown in Figure 4, the students can see the shift in structure and load on the specimen as it approaches and passes the yield point. (The dashed line and arrows highlight the relative atomic displacements associated with plastic deformation that have been superimposed on the image obtained from the simulation tool.) These images and computations have the potential to support learners' development of mental representations they can use to answer "what if" types of questions without use of the simulations, and then check their intuition by performing a detailed inquiry with a simulation.

From Lecture to Simulation Laboratory

The instructional initiative in this study began with two lecture sessions (here called Lecture and Prelab) designed to prepare students to independently manage their inquiry by using an MD

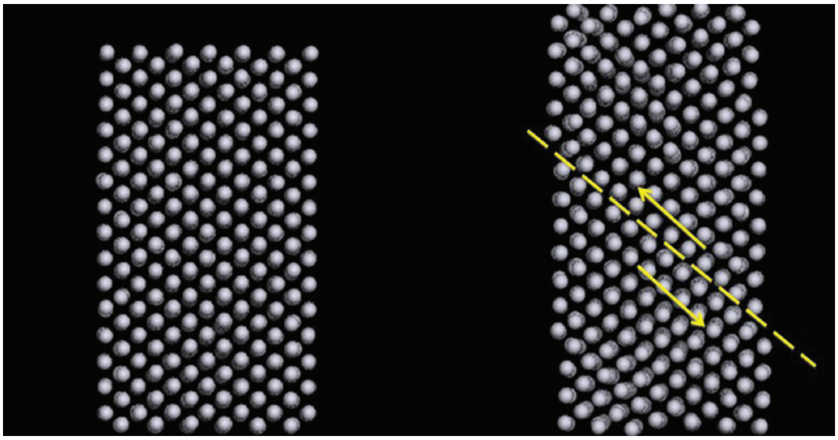

Figure 4. Visual illustration of a shift in structure under tensile loading.

simulation. The initial lecture (i.e., Lecture) provided students with background information describing the foundational concepts of mechanical principles and the theoretical foundations of the computational model governing the behavior of the MD simulation. Students are shown how Newton's equations of motion are used with an interatomic potential to predict the motion of every atom in a material. The second lecture (i.e., Prelab) provided an overview of how to perform MD simulations using the nanoMATERIALS tool at nanoHUB.org with details about setting various input conditions and describing important output representations the students might need to support their inquiry. The Prelab also compared and contrasted the macro-level experiment with the atomic-level experiments to highlight key features to look for from an expert perspective. Further, Figure 5 illustrates how the instructor explicitly highlighted this comparison of macro-level specimen with the empirical data of stress and strain and the pictorial image of the molecular structure model of the specimen. Through this demonstration, the instructor helped students structure their initial steps in their investigation and scaffolded their search through the array of outputs (10 possible choices of output representation) that will be most useful to their investigation during the Simulation Lab.

Our instructional initiative centers on coupling these traditional lectures and demonstrations with inquiry-based hands-on *virtual experiments* (online computer simulation modeling a physical experiment), which can lead to students' noticing more sophisticated governing principles defining properties of materials in the range beyond the yield point of the material. Moreover, the multiple outputs of a molecular dynamic simulation like those shown in Figure 5 can have great potential for supporting students' development of mental representations that they can use to predict results from conditions they have never previously experienced.

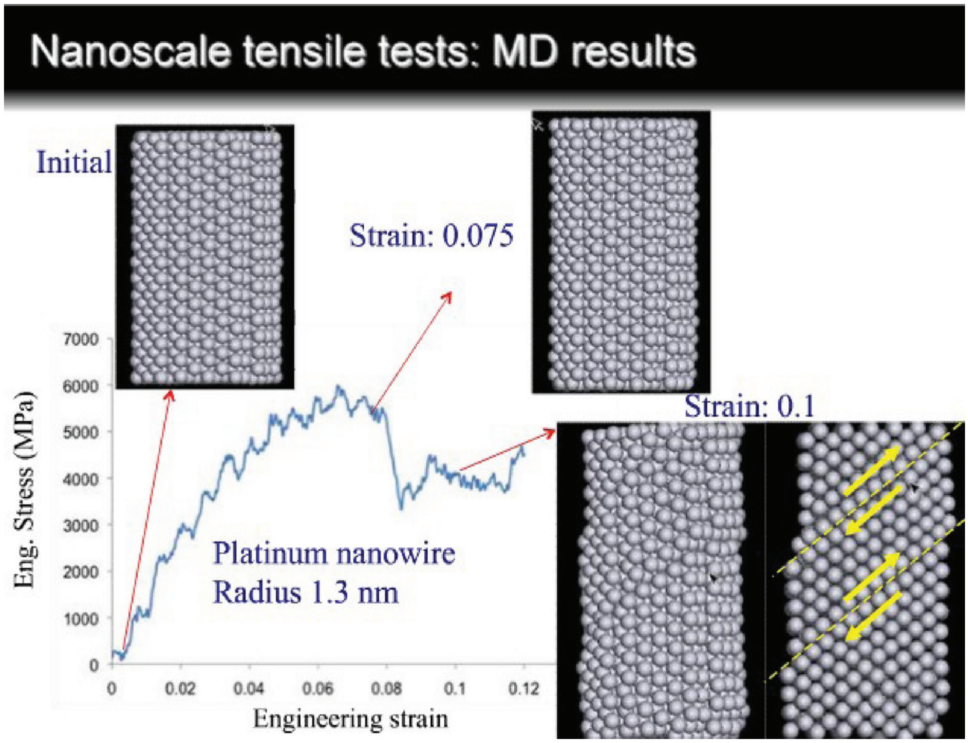

Figure 5. Mapping empirical data with a pictorial image of molecular structure.

APPROACH AND RATIONALE: A THEORETICAL PERSPECTIVE

Computational models and simulations in education

Computational modeling and interactive simulations can be powerful learning resources in all disciplines of science (Roberts, Feurzeig, and Hunter 1999) and engineering because these tools provide learners with methods to make invisible concepts visible and methods for articulating detailed explanations of complex ideas, such as Newton's laws of force and motion. Computational models "are based on mathematical algorithms that approximate fundamental laws and exhibit behavior that reproduces some important observed phenomena" (Pallant and Tinker 2004, 51). MD simulations involve the numerical solution of Newton's equations of motion for every single atom in a material with forces obtained from an interatomic potential or force field that describes how atoms interact with one another (Frenkel and Smit 2001; Strachan 2008; Park et al. 2010). The power of these tools depends on its ability to provide experimentally inaccessible insights into the behavior of materials (Brostow and Simoes 2005).

Theories of material behavior can be represented through spatial relationships of atoms to one another. This perceptual model can provide a learner with a mental representation of the atomic level system of atoms and how they interact with one another, which they can use to explain the observed properties of the material at the macro level. Also, mathematical models can provide a quantitative explanation for the absolute magnitudes of resulting forces and distances between the atoms. Together these visual and mathematical representations have the potential to provide a rich description of how a material will behave under the influence of an external load and illustrate the rearrangement of the system of atoms defining a material structure. Images like those in Figure 1–2 are excellent instructional tools used by textbook authors and instructors to explain material properties and the experimental tests performed to assess them (e.g., stress, strain, and yield strength) at the macro level. Perceptually, students can see critical events, like a material stretching and returning to original size before yielding, and then how a specimen permanently deforms after the yield point. Connecting the graph of stress and strain (quantitative model) with this perceptual model allows students to make sense of important descriptive characteristics for explaining how a material deforms with time. However, the macro-level description does not provide students with the mechanistic behavior describing why the material becomes harder in this range.

A series of images can help illustrate the atomic processes responsible for the material's response of interest, such as strain hardening of a material through plastic deformation. Figures 3 and 4 exemplify the concept of plastic deformation when an external force is applied to a nanowire. The use of images as part of didactic lectures is known to support learners' comprehension and recall of basic facts and concepts used to describe the features of a system (Mayer 2005, 2009). However, a learner's ability to mentally manipulate spatial models like these is not universal and requires the development of spatial skills and abilities (e.g., Schwartz and Black 1999; Hegarty et al. 2006). The expressive quality of simulation and visualization can support novice learners' comprehensions of difficult concepts and may help them develop more accurate mental representations of atomic-scale phenomena (Glenberg and Langston 1992; Hegarty and Just 1993). When students develop more accurate mental representations, they may demonstrate more expert reasoning about how a system behaves and be better able to predict changes through inductive reasoning (Chi, Glaser, and Farr 1988; Lehrer and Schauble 2006).

Several studies have investigated how people infer motion from static images (Hegarty 1992; Narayanan, Suwa, and Motoda 1994, 1995; Schwartz and Black 1996), or mental animations (Hegarty, Kriz, and Cate 2003) similar to the tasks students are asked to do with the MD simulation. The images from molecular dynamics simulation are analogous to the mechanical systems investigated in other cognitive studies on student developments of mental models. The models shown in

Figures 3, 4, and 5 become a base representation students can use to visualize how a system's structure will change over time; just as experience with a pulley system provides the background knowledge necessary to perform a mental animation. Further, their prediction of the new shape and their understanding of the forces supporting the structure help them to make appropriate predictions and explanations of various conditions they have not yet encountered as part of their instruction, either in lectures or in the simulation laboratory. This framework of mental representations is one of the primary learning mechanisms associated with students' sense-making of materials in different conditions. Other instructional factors are critical to increasing their abilities to make inferences about how materials will behave under a wide range of conditions (e.g., physical dimensions of material, temperature, and loading conditions).

Computational models can simulate the change of a system over time and generate animations that provide visual (spatial models) of how the system is changing. Therefore the output of the simulations provides critical *demonstrations* of how the system changes, which support students' development of their own mental models that they can use to predict how a new system will behave (Mayer 2005). The lecture activities used in our treatment provide this canonical view of the knowledge students are to acquire from the instruction.

Simulation laboratories provide students with the opportunity to engage in authentic learning experiences that require them to independently generate explanatory models they can use to make inferences. (Atkinson et al. 2000; Chi et al. 1989; Cannon-Bowers and Salas 1990). This mechanism for learning relates closely to the learning activities in the virtual laboratory experience following the prelaboratory lectures. The computational laboratory engaged learners in an inquiry activity designed to put them in an experimental process of evaluating characteristic changes in the output of the system (spatial relationships of atoms seen in visualization, e.g., Figure 3) with the input parameters they were controlling.

Designing to specific learning objectives

The instructional sequence for using the nanoMATERIALS Simulation Tool at nanoHUB.org transitioned learners from listening and observing examples of material properties being demonstrated with computational tools to self-guided discovery to explain how these materials change based on the governing principles of materials. Therefore the main objectives of this simulation-based learning module were to help students to (a) predict the change in the atomic structure of a material under various loading conditions, and (b) describe the relationship between the macro- and microlevel scales of a material after loading (e.g., explain strain hardening in terms of atomic structure and *why* the material is stronger, not just *that* it is stronger). In the following section we define the quasi-experimental method used to evaluate the potential of our instructional model. Our goal was to demonstrate an instructional model that leads to more robust conceptual understanding because it engages learners in a generative activity of running experiments to explain the trends observed in more-abstract graphs, as shown in Figure 5.

This process of exploration and explanation is critical to being able to transfer knowledge from one context to a new one. This study focused on identifying how well learners could transfer their knowledge explicitly targeted in a learning experience to a new condition founded on the same principles. Specifically transfer in their ability to predict the motion of atoms in a material in tension to a material in compression.

METHODS

Initially, this study was a design-based experiment (DBRC, 2003; Brown et al., 1991) to evaluate the appropriateness of the instructional approach, the benefits to learning, and the formative assessments we could use to inform the next implementation of the learning module. When we implemented the study, we had a split in our target population as a result their lack of participation in the lecture condition, which provided us a unique opportunity to achieve our original goals and also a comparison study of learning during two parts of the instructional method.

Our study was designed to investigate the value added by the prelab lectures and by a simulation laboratory using computational models with multiple visualization methods of data (e.g., material properties, stress versus strain) and spatial models of molecules (e.g., Figure 4 and 5). Based on prior experience and the literature, we expected the traditional lecture to reacquaint students with many of the fundamental facts and concepts associated with elastic and plastic deformation of metals they had learned about in prerequisite courses. We also expected that demonstrations with the simulation laboratory in lectures would not sufficiently provide a sophisticated model of material properties that would transfer to performing tasks, such as explaining and predicting how materials will change their structural properties at the atomic level when various control parameters are manipulated (e.g., temperature, applied force, and physical geometry). This premise is based on prior experience in teaching the course and other research on issues of transfer between learning conditions (Bransford and Schwartz 1999) and mechanisms for supporting cognitive development mentioned in the prior section. With additional work using the nanoMATERIALS Simulation Tool, students can explore the effects of temperature, size, and strain rate on the stress and strain relationship of nanoscale metallic wires. Their intuitions and development of the mental representation needed for explaining, and predicting the material behavior at the atomic level was expected to occur once they had engaged in the hands-on exploration of various materials for a range of conditions.

We expected that students would be able to explain the approximate orientation of slip planes and the slip direction in metallic samples subject to various loading conditions after participating in the Lecture, Prelab, and Simulation learning experiences.

Participants

The participants of this study included 46 sophomore materials engineering students enrolled in a course entitled Materials Structure and Properties Laboratories. They have completed several prerequisite courses that introduce many of the fundamental material properties taught during this course. Student groups were formed based on their self-selection to participate in the Lecture or Prelab, and all students participated in MD simulations. The study was not initially designed as a comparison study; however, the opportunity to evaluate for potential variance in the population because of the level of exposure to the learning materials was too important to ignore. Therefore the analysis separated learners into three categories: students who were (a) not present for Lecture and Prelab ($n = 6$); (b) present in either the Lecture or Prelab ($n = 16$); and (c) present in both, Lecture and Prelab ($n = 24$). All students participated in the Simulation laboratory.

Simulation-based learning module and procedures

The learning module was introduced during the Fall semester of 2009. Prior to this study, students were introduced to the mechanical response of polycrystalline metals to mechanical loading, and they analyzed several tensile tests on metallic specimens of various structures, compositions, and microstructures some also in polymeric samples. During these activities, the students were introduced to several topics regarding the mechanical response of metals, including strengthening mechanisms at an introductory level, as described in the course textbook. They were expected to understand (i) differences between elastic and plastic deformation; (ii) concept and definition of yield stress and work hardening; and (iii) obstacle-based strengthening mechanisms (solid solution, grain-size reduction, and strain hardening). As described earlier, the main objectives of this simulation-based learning module were to help students (i) explain the atomic processes governing plastic deformation, and (ii) begin to identify the difference in mechanical response between a nanoscale specimen and a macroscopic one. The learning module consisted of three major activities:

- Background **Lecture** (50 minutes) containing
  - Behavior of macroscopic samples in tensile loading
  - Behavior of a nanoscale wire stressing in tensile loading and the atomic mechanisms of inelastic deformation
  - Comparison of the behavior of material at macroscopic and nanoscale levels with empirical data representing relationship of stress and strain

- A **Prelab** lecture (50 minutes) containing
  - Review of goals and key concepts of the lab activities
  - Demonstration of how to use simulations in the nanoMATERIALS Simulation Tool on nanoHUB.org.
- MD **Simulation** laboratory (3 hours) where students
  - Use nanoMATERIALS Simulation Tool to simulate and observe deformation of a metallic nanowire, and then identify critical points of change in a material specimen and explain why (using first principles of mechanical physics) the deformation occurred as observed (guidelines provided in a laboratory handout)

The sequence of instruction was designed to build and expand students' comprehension of property-structure-process of materials, using computational models combined with traditional lecture and hands-on learning experiences. Table 1 outlines the sequence of activities and assessments. The pretest measure provides an indication of how well students learned during the two lectures, and the posttest measure allows us to quantify the value added of the hands-on simulation activities for achieving other learning objectives. Assessments A1 and A2 were identical.

Data collection and scoring methods

Three assessment items evaluated concepts the students explored during both the lecture and the hands-on activities. Students worked individually on the assessments with no external resources. The assessment contained three parts:

Yield stress (Q1): Asked students to compare the yield stress of a defect-free nanowire with that of a polycrystalline metal. This question is directly related to one of the objectives of the learning module, and its answer was given in the Lecture and Prelab; furthermore, this concept was reinforced by students performing the MD Simulation activities. This item was scored on a scale from 0 to 1 where 0 was given to incorrect answers, and 0.67 was given to students who correctly identify that a defect-free nanowire would be stronger, but who do not provide a correct justifications for this observation. One point was assigned to students who gave the correct answer, including a valid justification.

Lectures		Assessment 1 (A1)	MD Simulation Lab	Assessment 2 (A2)
Lecture (50 minutes)	Prelab (50 minutes)	Pretest (Posttest of lectures) (10 minutes)	Simulation (3 hours)	Posttest of entire sequence (10 minutes)

Table 1. Sequence of treatments and measures of student learning during the learning process

Plastic deformation in compression (Q2a) and plastic deformation in tension (Q2b): Asked students to sketch the atomic displacement involved during compressive (part a) and tensile (part b) plastic deformation of a nanowire. The answer to part b was given in the lectures and is specifically described as an activity found in the simulation lab. Answering part (a) required students to make an inference based on the results in tension. The scoring method applied for both Q2a and Q2b consisted of three possible responses. Zero was given if the response was incorrect; 0.5 the student correctly identified the slip plan, but had a wrong or missing slip direction; and 1 if the student correctly identified the slip plan and the slip direction.

Strain hardening (Q3): Asked students to compare the amount of strain hardening expected in the nanowire and the macroscopic samples (a cold-worked specimen and one that has been annealed). To correctly solve the problems, the students needed to understand that neither the nanowire nor the cold-worked sample can increase the density of dislocations, and thus they will exhibit no work hardening. Two possible scores were assigned for these multiple-choice questions. Zero was given if the response was wrong and 1 if students identified that neither the nanowire nor the cold-worked sample can increase the density of dislocation; therefore they will exhibit no work hardening.

This assessment instrument was designed to capture various levels of learning objectives associated with knowledge acquisition and transfer (Martin, Rivale, and Diller 2007). The first level targets *fact recall*, such as vocabulary and descriptive processes (e.g., Yield stress [Q1] and Strain hardening [Q3]). The goal was to help students become familiar with the formal language associated with explaining properties and structures of materials. These assessment items targeted student abilities to recall information mentioned in the activities. The second level targeted a more *conceptual* understanding of materials processes necessary to describe and explain the processes associated with plastic deformation (atomistic processes of plastic deformation in tension and compression [Q2a and Q2b]).

Each level of objectives was measured with various assessment formats. Appendix A provides the specific items used for this study. Measuring facts was accomplished with simple multiple choices

	Learning Activity		
Group	**Lecture**	**Prelab**	**Simulation**
1 (N=6)	No	No	Yes
2 (N=16)	Yes (or No)	No (or Yes)	Yes
3 (N=24)	Yes	Yes	Yes

Table 2. Definition of groups

and fill-in-the-blank answers. Students needed only to recall specific ideas in the appropriate context.

Data analysis methods

An initial step in the analysis was to group students according to the number of instructional activities they received: those who were (a) not present for Lecture and Prelab (n = 6); (b) present in either the Lecture or Prelab (n = 16); and (c) present in both, Lecture and Prelab (n = 24). All groups participated in the molecular dynamics simulation (nanoMATERIALS Simulation Tool), which began with Pretest and ended with Posttest.

Two analyses were performed on the pre-/post-tests. The first investigated the differences in three groups based on their pretest scores to evaluate the potential effects of Lecture or Prelab only. The initial step was to use composite scores for each group on the pre- and post-test and plot to determine if an interaction existed between the groups. The next step in the analysis used a contingency table and a proportional odds model to investigate differences within groups based on pretest scores. The proportional odds model used student condition as the explanatory variable, and pretest score as the response.

The second analysis investigated the effects of the MD Simulation experience using a comparative analysis of the pre- and post-test scores and whether there were differences between the three groups of students. An ANOVA model was used with condition as the explanatory variable (1) no background lecture, no prelab lecture; (2) background lecture or prelab lecture; and (3) background lecture and prelab lecture and the difference in the pre- and posttest scores as the response. By modeling the difference in test scores, we effectively blocked over each student, removing student-to-student variations. Using the ANOVA model, we looked for whether there was significant improvement from pre- to post-test scores for both the aggregate score and each item on the test. A Tukey Comparison adjustment was used to control the Type 1 error rate. Note that by modeling the difference, we possibly violated only one ANOVA assumption: the normality of the residuals. However, we did not feel it was severe enough to influence the findings because of the robustness of the model and because the normality assumption primarily affects predictions, which we did not do.

RESULTS

Overview of general effects

The Pretest measure was conducted after the Lecture and Prelab; therefore this measure could be used as a postmeasure of both lectures. Figure 6 illustrates a large difference in performance on the

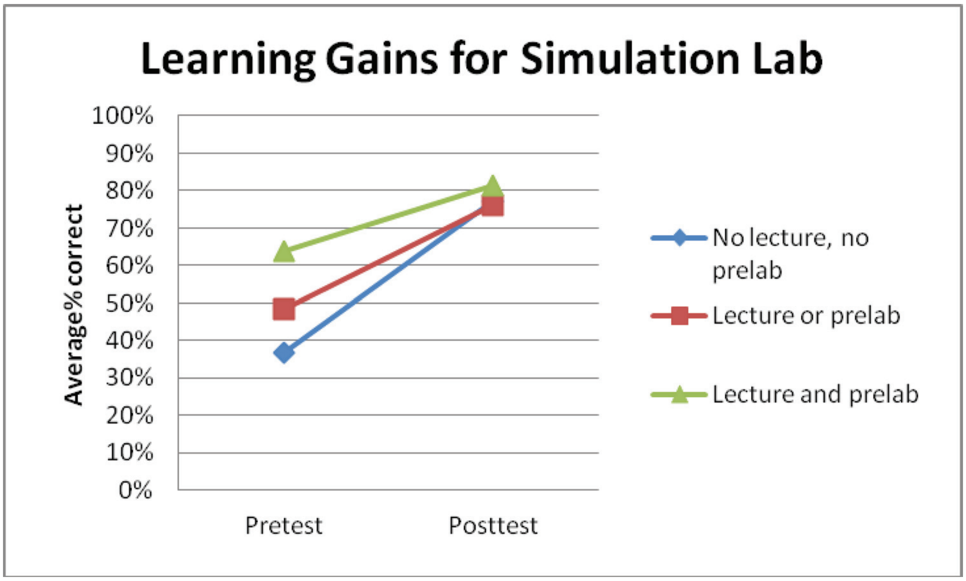

Figure 6. Learning from Lecture Series and Simulation Lab.

total score for all items. This difference suggests, as we expected, that participating in both lectures had a significant effect on students' learning of the basic concepts. Without a pretest measure for the lecture treatment, the results are weakened. However, conducting a simple comparison across the pretest items indicates that all the lectures have some effect on the students' learning of basic concepts, and for all students there is room for improvement (the best scores are still below 65%). Figure 7 illustrates student pre-/post performance on individual items and graphically shows the difference between groups at each event. Item Q2a, focused on the transfer of conceptual understanding of plastic deformation in compression, had a very low average for all students. As we hypothesized, question Q2a (transfer question) required additional knowledge that the learners needed, but the lectures did not directly provide it. A Chi-Squared analysis (discussed later in Table 7) indicates that there is no significant difference between the groups for Q2a on the pretest, but there was a significant difference between the remaining items. The performance on item Q2a could support the assumption that students have similar background knowledge about properties of materials at the beginning of this treatment series of lectures and simulation laboratories. Furthermore, the Lecture Series provided no additional background knowledge necessary to answer item Q2a.

Figure 6 also illustrates the gain in students' performance after the Simulation experience. Potential explanations for this could be that students who participated in all the treatments showed a stronger understanding of the context for questions asked because they were relevant to the

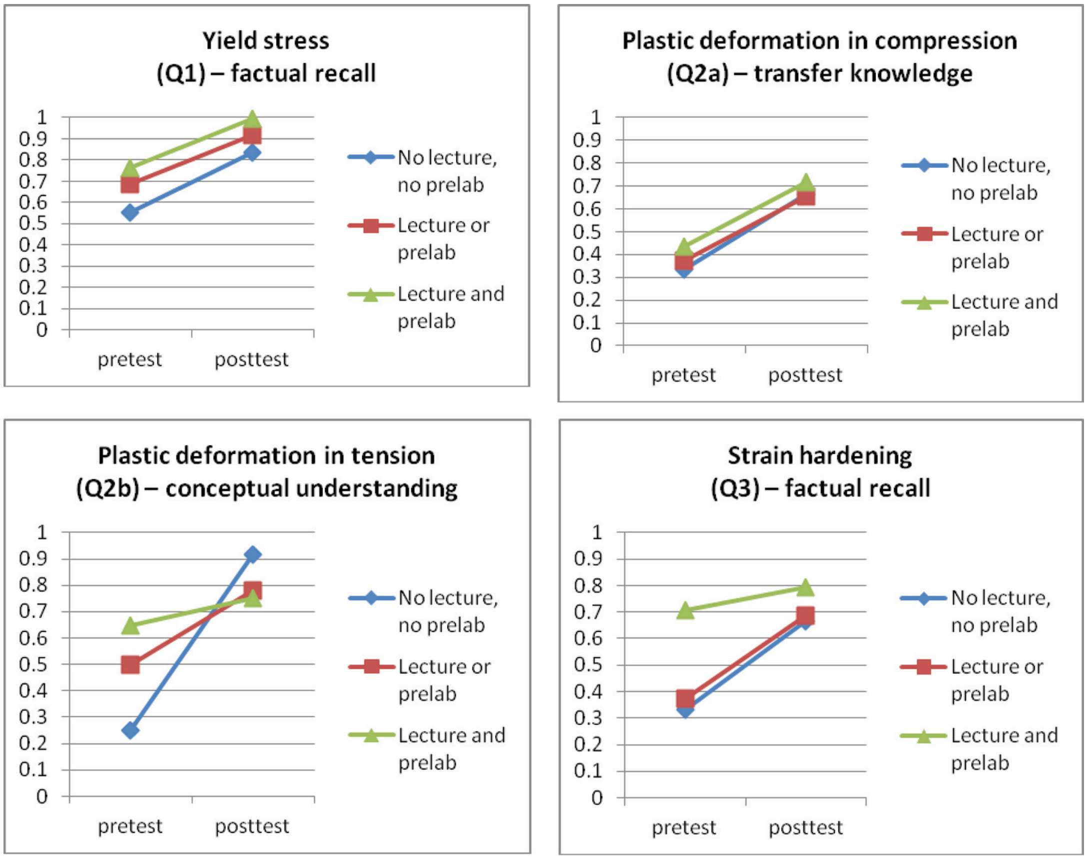

Figure 7. Value-added of Simulation Laboratory

previous lectures. The students who did not participate in the lectures had little time to recall and organize their thinking about prior concepts they knew. However, once they participated in the lab, they may have been better prepared to make sense of the Simulation experiences. Also, we know little about the inquiry process used by these students as they interacted with the simulation.

In general, all students achieved very similar performance levels even if they did not participate in the Lecture or Prelab. The variance of the students can potentially be explained by observing which ones participated in lectures containing general background and prelaboratory discussion about materials and testing methods. The overall scores illustrate how all students progressed in their performance on the posttest. Further, the value-added of the Simulation can be observed across all groups. The following summary of results provides a more detailed quantitative analysis of these results.

Item analysis of Pre-/Post measure

The indicated increase in average scores shown in Figure 6 suggest that students who were exposed to more direct instruction from the Lecture or Prelab performed better on the pretest measure. For each items we compared between groups on the pretest. Fisher's Exact Test results showed that for questions Q1, factual recall of yield stress ($p = 0.02$), Q2b, conceptual understanding of plastic deformation in tension ($p = 0.04$), and nearly for Q3 factual recall of strain hardening ($p = 0.07$), there was significant difference between the three groups. This would be consistent with the assumption that lectures provided background knowledge that prepared students to answer these kinds of questions.

In regard to Q2a, transfer of conceptual understanding of plastic deformation in compression, ($p = 0.16$), student performance was not significantly different among the conditions for the pretest. Note that question Q2a is a transfer question and was not explicitly covered in the Lecture or Prelab; therefore, the lectures alone did not prepare learners to transfer what the learned in the lecture to a new condition

Table 7 reports the results of the proportional odds model. These results are the same as Fisher's Exact Test for the contingency tables, showing significant differences in pretest scores for the three different conditions for Q1, Q2b, and Q3.

Comparing participants' responses between the pretest and posttest, the least square means analysis revealed that use of the simulation tool resulted in significant post score improvement for factual recall in identifying yield stress (Q1) as shown in Table 8. The results shown in Table 9 revealed a similar result for the transfer of conceptual understanding of plastic deformation in compression (Q2a). For identifying conceptual understanding of plastic deformation in tension (Q2b), the no-Lecture and no-Prelab condition and the Lecture or Prelab condition resulted in significantly improved performance in the posttest scores, as shown in Table 10. Lastly, ANOVA results for the

Condition	0	0.67	1	Total
No Lecture, no Prelab				
Frequency	1	5	0	6
Percent	17%	83%	0%	100%
Lecture or Prelab				
Frequency	1	12	3	16
Percent	6%	75%	19%	100%
Lecture and Prelab				
Frequency	3	8	13	24
Percent	13%	33%	54%	100%

Table 3. Percentages by Pretest for factual recall of yield stress (Q1)

Condition	0	0.5	1	Total
No lecture, no Prelab				
Frequency	3	2	1	6
Percent	50%	33%	17%	100%
Lecture or Prelab				
Frequency	6	6	3	16
Percent	44%	37%	19%	100%
Lecture and Prelab				
Frequency	5	17	2	24
Percent	21%	71%	8%	100%

Table 4. Percentages by Pretest for transfer of conceptual understanding of plastic deformation in compression (Q2a)

conceptual understanding of strain hardening (Q3) revealed a significant improvement in test scores for students in the Lecture or Prelab condition only (see Table 11), with no significant difference between the groups. Finally, we performed a Chi-Squared analysis on posttest scores for question Q2b that revealed no significant difference across the three groups ($p = 0.2708$).

DISCUSSION

In this study, we hypothesized that undergraduate engineering students can use research grade simulation tools to develop their conceptual understanding of how a system works and the magnitude of factors that govern how that system behaves. As expected, the lectures provided students with knowledge of basic facts and concepts they could recall, and the simulation laboratory supported students' conceptual understanding needed to analyze novel contexts. The pretest results illustrated how a lecture is necessary for the students to perform well on questions associated with facts and basic definitions of concepts. Using the no-lecture group as a control condition, it is clear that attending the lectures provided the necessary background to answer certain items on the test (factual questions and replication questions seen in prior instructor lead discussions/classes). The experience may have also provided them with knowledge to be more autonomous in their inquiry; however, this study has insufficient data to warrant this claim.

This comparative analysis assumed that all students were similar in their abilities. Some evidence to support this assumption is their comparative performance on item Q2a, transfer of conceptual

Condition	0	0.5	1	Total
No lecture, no Prelab				
Frequency	4	1	1	6
Percent	66%	17%	17%	100%
Lecture or Prelab				
Frequency	3	10	3	16
Percent	19%	62%	19%	100%
Lecture and Prelab				
Frequency	2	13	9	24
Percent	8%	54%	38%	100%

Table 5. Percentages by Pretest for conceptual understanding of plastic deformation in tension (Q2b)

Condition	0	1	Total
No lecture, no Prelab			
Frequency	4	2	6
Percent	67%	33%	100%
Lecture or Prelab			
Frequency	10	6	16
Percent	63%	38%	100%
Lecture and Prelab			
Frequency	7	17	24
Percent	29%	71%	100%

Table 6. Percentages by pretest for factual recall of strain hardening (Q3)

understanding of plastic deformation in compression. Also all the students are at the same point in the curriculum at an institution with high academic standards. Item Q2a on the pre-/post-test had no direct instruction associated with the answer. Therefore, all students were in the same condition of needing to generate new knowledge to answer the questions correctly, since the performance across all groups is similar for this item on the pretest. Further, students who did not attend the lecture are capable of learning quickly, as indicated by their strong overall performance on the post assessment. The lack of an overall pretest before lectures weakens the claims about the effect of the lectures on learning, and the logical argument for homogeneity of the students helps to illustrate the effect of the MD Simulation, which is the primary focus of inquiry for this study.

Question	Maximum Likelihood Estimate	Pr > ChiSq	Odds Ratio Estimate
Yield stress (Q1) – factual recall	1.0408	0.0204	2.831
Plastic deformation in compression (Q2a) – transfer of conceptual understanding	0.4168	0.3079	1.517
Plastic deformation in tension (Q2b) – conceptual understanding	1.1887	0.0077	3.283
Strain hardening (Q3) – factual recall	0.9761	0.036	2.654

Table 7. Proportional Odds Estimate for all questions in the pretest

Condition	Difference post-pre	Standard Error	DF	T value	Pr > |t|
No Lecture, no Prelab	28%	0.1395	43	1.99	0.0528
Lecture or Prelab	23%	0.08542	43	2.68	0.0103
Lecture and Prelab	23%	0.06974	43	3.29	0.0020

Table 8. Least Squares Means for factual recall of yield stress (Q1)

The simulation lab increased most students' understanding of facts, concepts, and synthesis skills beyond the instruction provided by the lecture activities. An important finding is the increased performance by all groups on question Q2a, aiming to identify conceptual understanding of plastic deformation in compression. This item was a novel question not directly taught as part of the Lecture or Prelab presentations or an inquiry activity with the MD Simulation. The low performance on the pretest of all students on this transfer item suggests that the lectures alone do not provide the knowledge they need to successfully transfer what they learned. Yet the major increase in students' performance occurred from the inquiry-based activities with the MD Simulation experience. The assessment item targeted their abilities to sketch the atomic processes caused by plastic deformation induced by the application of different external conditions (compressive versus tensile forces). Since students' abilities to draw these images increased across the treatment, the results suggest that their abilities to comprehend these spatial relationships and to predict behavior came as a direct result of interacting with the visual animations provided by the nanoMATERIALS Simulation Tool.

The findings of this study have important implications for engineering education, especially for domains where direct observation of a phenomenon is challenging, as nanotechnology is. This experiment clearly demonstrates the potential for engaging learners through "hands-on" activities that lead

Condition	Difference post-pre	Standard Error	DF	T value	Pr > |t|
No Lecture, no Prelab	33%	0.1554	43	2.14	0.0377
Lecture or Prelab	28%	0.09517	43	2.96	0.0051
Lecture and Prelab	28%	0.07771	43	3.62	0.0008

Table 9. Least Squares Means for transfer of conceptual understanding of plastic deformation in compression (Q2a)

Condition	Difference post-pre	Standard Error	DF	T value	Pr > |t|
No Lecture, no Prelab	67%	0.1383	43	4.82	<.0001
Lecture or Prelab	28%	0.08467	43	3.32	0.0018
Lecture and Prelab	10%	0.06913	43	1.51	0.1392

Table 10. Least Squares Means for conceptual understanding of plastic deformation in tension (Q2b)

Condition	Difference post-pre	Std. Error	DF	T value	Pr > |t|
No Lecture, no Prelab	33%	0.2027	43	1.64	0.1074
Lecture or Prelab	31%	0.1241	43	2.52	0.0156
Lecture and Prelab	8%	0.1014	43	0.82	0.4156

Table 11. Least Squares Means for factual recall of strain hardening (Q3)

to increased conceptual understanding of how the atomic structure of a material changes under various conditions. Conceptual understanding may be associated with facts, but deeper conceptual understanding is associated with visualizing models to comprehend and predict behavior of the system. We believe the mechanisms of visualizations described in the literature were the same mechanisms associated with the increased performance of these students. We expect to conduct additional studies using qualitative methods to better explore the conjectures associated with how students learn with simulations, in particular those linked with engineering contexts such as design or analysis of materials properties.

This study had several limitations that reduce the claims that can be made about the learning potential of the lecture treatment. First, we assumed that participating students possess similar prior knowledge and skills about materials properties because all students successfully completed prerequisite courses and are all first semester second-year undergraduate students. Also, all students performed equally well on the posttest, suggesting that students who chose not to participate in the lectures were competent learners. However, the quasi-experimental design could be strengthened with the addition of another covariant measure, such as a pretest or the use of students' grade-point average.

Similarly, the assessment was designed primarily to evaluate the achievement of the learning goals for the MD Simulation and not the lectures directly. The assessment would need to be expanded to include additional measures that would test such things as student abilities to recall various facts presented in lectures to explain the mathematical foundation of the model used in the simulation. The lectures also provide background information students would need to simply use the MD simulation tool and to make sense of the outputs from simulations. We have no systematic data to evaluate if students who did not attend lectures also had difficulties using the simulation tool. One possible outcome would be that students were not well prepared to participate in the lab and therefore lost a significant amount of start-up time before they engaged in the inquiry activity. Also, without the background knowledge provided by the lectures, the no-lecture students may have required more assistance by the instructor, or may have been frustrated because of their lack of knowledge.

A future study would include additional controls, assessments, and evaluations of students' inquiry processes during the laboratory experience to capture an even richer description of the value-added by this instructional sequence. We would envision working with a similar population of students with increased sample size. If possible, a cohort of students in the general science would be an interesting comparison group. The new pre/post measure would include items to capture knowledge and skills unique to the lecture and the MD simulation lab. Observational measures of the classroom interaction would be used to capture the types of interactions between the students and instructor during all the sessions. Similarly controlled studies of students interacting with the visualization would increase our understanding of how students processed information provided the MD simulation. Finally, at the end of the intervention students would be asked to complete a self-report of their perception of their learning and the strengths and weakness of the instructional approach.

CONCLUSION

This study corroborates previous findings identifying molecular dynamic simulations as powerful tools to convey concepts related to atomic-scale phenomena. In particular, these results show that hands-on atomistic simulations not only helped students better understand the behavior of the specific conditions they simulated, but also helped them to transfer that knowledge to the behavior of macroscopic samples seen previously during the course. The results from this performance assessment suggest that simulation experience alone is equivalent to learning associated with both Lecture and Prelab. Several additional learning outcomes can be achieved with the lecture, including issues of retention of information and ability and overall engagement level of the students in the various groups. Those who participated in all the lectures may have been better prepared to engage the simulations with an inquiring mind. They may have explored more concepts that were not part of the assessment. They may have approached the activities with more confidence, and they may have generated more interest in the domain. All of these factors are additional parameters to be evaluated in further studies.

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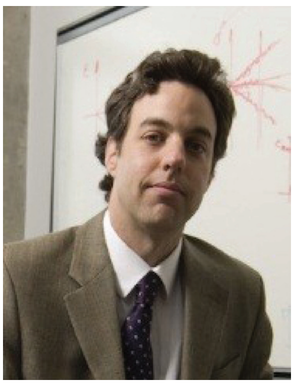

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